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NARROW GAP HgCdTe ABSORPTION BEHAVIOR NEAR THE BAND EDGE INCLUDING NONPARABOLICITY AND THE URBACH TAIL (POSTPRINT)

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An analytical model describing the absorption behavior of HgCdTe is developed that simultaneously considers the contributions from nonparabolic conduction and light hole bands as calculated by a 14 x 14 matrix $k\cdot p$ method as well as the Urbach tail. This model is capable of smoothly fitting experimental absorption coefficient curves over energies ranging from the Urbach tail region to the intrinsic absorption region up to 300 meV above the band gap. Comparisons to the experimental results give good agreement.

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Narrow gap HgCdTe absorption behavior near the band edge including nonparabolicity and the Urbach tail

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An analytical model describing the absorption behavior of HgCdTe is developed that simultaneously considers the contributions from nonparabolic conduction and light hole bands as calculated by a 14×14 matrix $k\cdot p$ method as well as the Urbach tail. This model is capable of smoothly fitting experimental absorption coefficient curves over energies ranging from the Urbach tail region to the intrinsic absorption region up to 300 meV above the band gap. Comparisons to the experimental results give good agreement. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2245220]

The HgCdTe absorption coefficient as a function of absorbed photon energy in the vicinity of the optical energy gap E_0 has two major regions: (1) below E_0 it follows Urbach's rule, describing transitions between localized band-tail states, and (2) above E_0 to approximately 300 meV over E_0 (hence far below the next critical point in the absorption structure), called the intrinsic or Kane region, describing transitions between extended valence and conduction band states. Modern HgCdTe detectors with advanced architectures usually employ devices with thin absorber layers, so the cutoff wavelength is determined by photons with high absorption coefficients (up to 10^4 cm^{-1}), a region where previous models[1,2] using parabolic approximations have shown significant deviations from experimental data.

HgCdTe samples were grown on CdZnTe substrates in a Riber 32P molecular beam epitaxy system. The high material quality, high composition, and thickness uniformity both along[3] and perpendicular[4] to the growth direction, and the optically good flatness of HgCdTe epilayers enable reliable measurement of the absorption coefficient over the 10^2–10^4 cm^{-1} range, which covers both the Urbach tail and intrinsic absorption (up to 300 meV) regions. The details of the growth procedure are discussed elsewhere.[5,6] The samples are n-type (low 10^{15} cm^{-3}), with visible surface defects such as craters,[7,8] voids, and microtwins less than mid-10^3-cm^{-2} in density and threading dislocation densities in the low 10^5 cm^{-2} as revealed by etch pit density measurements using Schaake's etchant.[9] They are selected to be representative of standard n-type absorber region of typical photodiodes. Infrared transmission measurements were performed as described in detail elsewhere.[10]

Previous works[2,10–12] have demonstrated that the absorption coefficient of HgCdTe below optical energy gap E_0 can be fitted by the formula suggested by Urbach[13] as follows:[14]

$$\alpha = \exp[(\hbar\omega - E_0)/W] = \alpha_0 \exp(\hbar\omega/W), \tag{1}$$

where $\hbar\omega$ is the absorbed photon energy, α_0 is the absorption coefficient at the energy of E_0, and W is the Urbach energy. The Urbach absorption tail energy has been discussed elsewhere in detail.[10] It may vary from sample to sample and also from area to area within the same sample, as revealed by infrared microscope mapping.[15]

The Kane model[16] is the most commonly used model to describe the band structure near the Γ point of narrow gap semiconductors with nonparabolic bands. The energy-momentum relationships of conduction band $[E_c(k)]$ E_c can be written in the hyperbolic form

$$E_c = \sqrt{s^2k^2 + b^2} - b + E_g, \tag{2}$$

where $b=E_g/2$ and $s=\pm\sqrt{2P^2/3}$ are the slopes of the two asymptotes. k is the electron crystal momentum, E_g is the energy band gap, P is the momentum matrix element with a value of $(8.0–8.5)\times10^{-8}$ eV cm.[17,18]

More precise $k\cdot p$ calculations using a 14×14 matrix[19] give similar hyperbolas describing the E_c or E_{lh} dispersions. Figures 1(a)–1(c) show 14×14 $k\cdot p$ calculated results as well as fitting to Eq. (2) for $Hg_{0.77}Cd_{0.23}Te$ at the temperature of 77 K. s and b act as two parameters describing the shape of both conduction and light hole bands because these two bands are symmetric. Specifically, E_c fits give $s=8.85\pm0.01$ ($\times10^{-8}$ eV cm) and $b=103\pm2$ (meV). Similar results for HgCdTe with a similar composition at 0 K were also obtained by Krishnamurthy *et al.*[20] The asymptotes can be used to approximate the E_c dispersion relationship when E or k is large. On the other hand, when k is small, the lowest order term of a Taylor series of Eq. (2) will give a reasonable approximation:

$$E_c = E_g + \frac{s^2}{2b}k^2, \tag{3}$$

which describes a parabolic E_c dispersion relationship near the Γ point, as shown in Fig. 1(c). The electron effective

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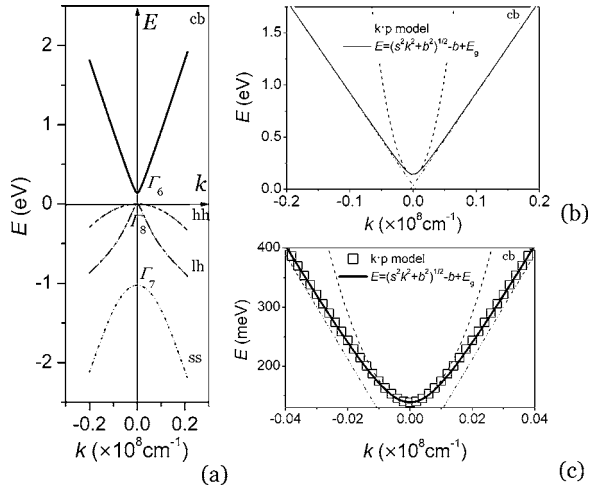

FIG. 1. (a) Energy band structure of $Hg_{0.77}Cd_{0.23}Te$ near the Γ point at 77 K calculated using a 14×14 matrix $k\cdot p$ method. Solid line: conduction band; dashed line: heavy hole band; dash-dotted line: light hole; and dash-dot-dotted line: split-off band. (b) Open circles: calculated results from (a) for the conduction band; solid line: fitted Eq. (2) in text; dash-dot-dotted line (this is visible only near $k=0$): high energy asymptotes of hyperbola; and dashed line: fitted parabola, which deviates substantially from the other curves at higher energies. (c) Close-up of (b) near the bottom of the conduction band. Solid line: fitted using a hyperbola, which shows reasonably good agreement even at the bottom of the conduction band; and dashed line: fitted using a parabola, which shows good agreement only very near the band gap. The dash-dot-dotted lines are asymptotes of the hyperbola.

mass is obtained from $m_e^*/m_0=\hbar^2 b/s^2 m_0$, m_0 is the free electron mass.

Noting that the optical matrix elements vary slowly with k and restricting our attention to energies near the band gap (-20 meV$\leqslant\hbar\omega-E_g\leqslant400$ meV), we discuss the absorption behavior assuming that the optical matrix elements can be treated as constant. The absorption coefficient is

$$\alpha=\frac{A}{\hbar\omega}\cdot\rho_{CV}(k), \tag{4}$$

here A is a constant, and ρ_{CV} is the joint density of states, which can be rewritten as

$$\rho_{CV}(k)=\frac{K^2}{\pi^2}\left(\frac{\partial E_c}{\partial K}-\frac{\partial E_j}{\partial K}\right)^{-1}\Bigg|_{E_c(K)-E_j(K)=\hbar\omega}, \tag{5}$$

where K_j are the values of one dimension electron crystal momentum that fit the conditions $E_c(K_j)-E_j(K_j)=\hbar\omega$; j represents the light or heavy hole bands. Therefore, the total absorption coefficient α, which is the sum of absorption coefficients involving light hole ($\alpha_{\rm lh}$) and heavy hole ($\alpha_{\rm hh}$) bands, can be given as a function of $\hbar\omega$ or $\varepsilon=\hbar\omega-E_g$:

$$\alpha_{\rm hh}=\frac{A}{\pi^2(\varepsilon+E_g)}\cdot K_{c\text{-hh}}\cdot\left[\frac{s^2}{\sqrt{s^2K_{c\text{-hh}}^2+b^2}}+\frac{\hbar^2}{m_{\rm hh}^*}\right]^{-1}. \tag{6a}$$

$K_{c\text{-hh}}$ as a function of ε can be obtained by solving the following equation:

$$\varepsilon=\sqrt{s^2K_{c\text{-hh}}^2+b^2}-b+\frac{\hbar^2}{2m_{\rm hh}^*}K_{c\text{-hh}}^2. \tag{6b}$$

Let $\varepsilon_c=\sqrt{s^2K_{c\text{-hh}}^2+b^2}-b$ and $\varepsilon_{\rm hh}=(\hbar^2/2m_{\rm hh}^*)K_{c\text{-hh}}^2$; then $\varepsilon_c+\varepsilon_{\rm hh}=\varepsilon$ and ε_c and $\varepsilon_{\rm hh}$ correspond to the same electron crystal momentum $K_{c\text{-hh}}^2$. Because of the big difference between the electron and hole effective masses, it is a good approximation to set $\varepsilon=\varepsilon_c$. Then Eq. (6a) can be rewritten as

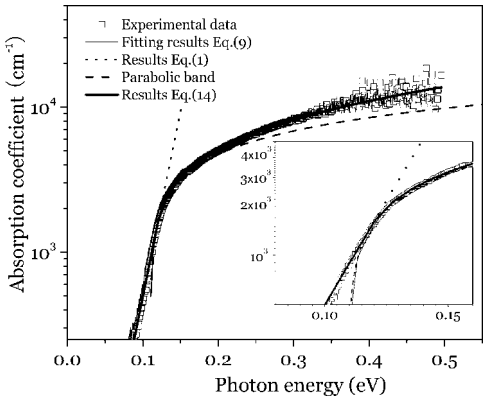

FIG. 2. Open squares: experimentally measured absorption coefficient of a $Hg_{0.79}Cd_{0.21}Te$ sample at 80 K; thin solid line: fitted Eq. (9) by assuming hyperbolic bands; dotted line: fitted Urbach tail [Eqs. (1) and (13) in text] dashed line: fitted assuming parabolic bands; and thick solid line: fitted using Eq. (14). The insert is a close-up of the main figure and shows that Eq. (14) remains smooth at E_0.

$$\alpha_{\rm hh}=\frac{A}{\pi^2s^3(\varepsilon+E_g)}(\varepsilon+b)\sqrt{(\varepsilon+b)^2-b^2}. \tag{7}$$

Because the conduction and light hole bands are symmetrical in the energy range of 400 meV beyond the band gap, we get

$$\alpha_{\rm lh}=\frac{A}{\pi^2s^3(\varepsilon+E_g)}\left[\frac{1}{8}(\varepsilon+2b)\sqrt{(\varepsilon+2b)^2-(2b)^2}\right]. \tag{8}$$

Therefore the total absorption coefficient above E_0 as a function of absorbed photon energy $\hbar\omega$ is

$$\alpha=\alpha_{\rm hh}+\alpha_{\rm lh}=\frac{B}{\hbar\omega}\left[(\hbar\omega-E_g+b)\sqrt{(\hbar\omega-E_g+b)^2-b^2}+\frac{1}{8}(\hbar\omega-E_g+2b)\sqrt{(\hbar\omega-E_g+2b)^2-(2b)^2}\right]. \tag{9}$$

Note that $B=A\pi^{-2}s^{-3}$ is a constant.

Equation (9) was used to fit the experimentally measured absorption coefficient for a $Hg_{0.79}Cd_{0.21}Te$ sample at 80 K; the results are shown in Fig. 2. When the photon energy is much larger than the absorption edge, Eq. (9) can be rewritten as

$$\alpha=\frac{C(\hbar\omega-E_g+D)^2+F}{\hbar\omega}, \tag{10}$$

where $C=9A/8s^3\pi^2$, $D=(10/9)b$, and $F=(A/9s^3\pi^2)b^2$. Note that the product of the absorption coefficient and the energy ($\alpha\hbar\omega$) goes as the square of the energy when the energy is greater than E_g by hundreds of meV. Equation (10) can also be obtained if one substitutes the $E_c(k)$ and $E_{\rm lh}(k)$ relations by the asymptote of Eq. (2).

Within about 20 meV of the energy gap, $\varepsilon=\hbar\omega-E_g\ll b$. Equation (10) can then be rewritten as

$$\alpha=\frac{Ab^{3/2}}{\pi^2s^3(\hbar\omega)}\left[\sqrt{2}+\frac{1}{2}\right]\cdot\sqrt{\hbar\omega-E_g}. \tag{11}$$

In fact, when ε or k is small, Eq. (2) can be used as an approximation of $E_c(k)$ and $E_{\rm lh}(k)$, and Eq. (11) can be derived as well. An example is shown in Fig. 2. An empirical formula with a similar form has been suggested by Scha-

cham and Finkman[21] from absorption very near the band gap in samples with thicknesses of 25–300 μm.[2]

Equations (9)–(11) give a clear picture of the changing tendency of $\alpha\cdot\hbar\omega$ with $\hbar\omega$, which can be combined into the formula $\alpha\cdot\hbar\omega\propto\varepsilon^{f(\varepsilon)}$, where $f(\varepsilon)$ is a function of ε taking the values of 0.5–2. $f(\varepsilon)=0.5$ when ε is very small. With increasing ε, $f(\varepsilon)$ gradually increases. When ε is very large, $f(\varepsilon)$ takes the value of 2. Therefore, depending on the range of energy above the band gap, an empirical formula of $\alpha\cdot\hbar\omega\propto\varepsilon^{\gamma}$ $(0.5\leqslant\gamma\leqslant2)$ can be used to describe the energy dependence of the absorption coefficient near the band gap, where $\gamma=(1/n)\Sigma_n f(\varepsilon_i)$, i.e., an average over n energy points taken into account during the fitting calculations above E_g. Such a result can also be derived from Eq. (5) through assuming dispersion relationships $E_c(k)=k^{3/(1+\gamma)}+E_g$ and $E_{\mathrm{lh}}(k)=-k^{3/(1+\gamma)}$. As shown in Fig. 1(c), such assumptions are reasonably correct as long as $1\leqslant3/(1+\gamma)\leqslant2$, corresponding to $0.5\leqslant\gamma\leqslant2$, being exactly the same range as in our previous discussions. Moazzami *et al.*[22] have empirically determined a γ value of about 0.7 for a $Hg_{0.69}Cd_{0.31}Te$ sample in the energy range of about 100 meV. Chu and co-works[12,23] found that a logarithmic approximation works best in the energy range of 100 meV above the energy gap.

The absorption coefficient below the energy gap is expected to follow the Urbach rule. As a semiempirical approach to guarantee a smooth connection, we require

$$\alpha_U|_{\hbar\omega=E_0}=\alpha_I|_{\hbar\omega=E_0},\quad \left.\frac{d(\alpha_U)}{d(\hbar\omega)}\right|_{\hbar\omega=E_0}=\left.\frac{d(\alpha_I)}{d(\hbar\omega)}\right|_{\hbar\omega=E_0}. \tag{12}$$

Then we obtain from Eq. (12) the condition

$$E_0\cong E_g+\frac{W}{2}. \tag{13}$$

Recall E_0 is the point where the absorption coefficient transitions from Urbach's rule to the intrinsic band-to-band behavior. E_0 was defined as the optical energy band gap of HgCdTe by Chu *et al.*[24] The first derivative of the absorption coefficient peaks at E_0.[17,25] Similar suggestions were made by Ariel *et al.*[26,27]

The combination of Eqs. (1), (9), and (13) gives the absorption coefficients near the band gap E_g as

$$\begin{aligned}\alpha(\hbar\omega)&=\frac{B}{E_g+W/2}\left[\left(\frac{W}{2}+b\right)\sqrt{\left(\frac{W}{2}+b\right)^2-b^2}\right.\\&\left.+\frac{1}{8}\left(\frac{W}{2}+2b\right)\sqrt{\left(\frac{W}{2}+2b\right)^2-(2b)^2}\right]\\&\cdot\exp\left(\frac{\hbar\omega}{W}\right)\qquad\left(\hbar\omega\leqslant E_g+\frac{W}{2}\right),\\&=\frac{B}{\hbar\omega}\left[(\hbar\omega-E_g+b)\sqrt{(\hbar\omega-E_g+b)^2-b^2}+\frac{1}{8}(\hbar\omega\right.\\&\left.-E_g+2b)\sqrt{(\hbar\omega-E_g+2b)^2-(2b)^2}\right]\\&\left(\hbar\omega\geqslant E_g+\frac{W}{2}\right).\end{aligned} \tag{14}$$

Here E_g is the band gap of HgCdTe and W is the Urbach tail energy in the same unit of E_g, and the parameters of b and B as functions of temperature and Cd composition in HgCdTe can be determined by fitting experimental data. This formula is plotted in Fig. 2 for an $x=0.21$ $Hg_{1-x}Cd_xTe$ sample at 77 K and gives good agreement with experimental data both below and above E_0.

In conclusion, an analytical model describing the absorption behavior of long wavelength infrared HgCdTe as a function of absorbed photon energy was established based on $k\cdot p$ band structure calculations. The model is capable of describing both the Urbach tail region and intrinsic region up to hundreds of meV above the band gap. The intrinsic band-to-band absorption coefficient is proportional to $(\hbar\omega-E_g)^{\gamma}$ with γ increasing from 0.5 and 2 with increasing photon energy, a consequence of the nonparabolic conduction and light hole band dispersion relationships. Good agreement was found between the experimental and theoretical results.

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